Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)
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Lead Institution: The Ohio State University
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***Mission Statement**: To understand the fundamental mechanisms of waste form performance and apply that understanding to design new waste forms with improved performance.*

WastePD will develop innovative approaches and solutions through the synergistic interactions of individuals who are experts in the degradation behavior, modeling, and design of glasses, ceramics and metal alloys. WastePD is the first center ever created to address the degradation of this diverse group of materials in a comprehensive and coordinated manner. The science goals are grouped into three common topics: corrosion mechanisms via advanced characterization, environmental impacts, and materials design. The fundamental understanding of the degradation mechanisms of the waste forms and containers will allow DOE to develop new materials with improved properties, to prevent environmental contamination and to explore totally new disposal concepts. The waste forms of interest are tank waste transformed into glass, ceramic materials containing radionuclides, and metal canisters that protect the various waste forms.

The synergistic activities between the materials classes in the areas of experimental techniques, computational methodologies, and design approaches are a key component of WastePD. These synergistic activities will stimulate the achievement of new discoveries and reveal physical insights that would otherwise have been overlooked or not recognized. Sharing the understanding of the degradation mechanisms of glasses, ceramics, and metal alloys will lead to identification of commonalities and new materials design rules.

Glass Projects

DOE's Office of Environmental Management (EM) currently manages high-level wastes stored in underground tanks that have already begun to leak. This waste will be immobilized as borosilicate glass before disposal. Accurate prediction of the performance of a disposal facility therefore requires understanding and control of waste glass corrosion over geologic time-scales. This remains a major challenge because of the very slow reactions that occur between two unstructured media that are far from equilibrium (glass and gel). Additionally, a series of coupled processes occurring at the nexus between water being the solvent and water being a solute are responsible for the overall rate of glass water reactions. It is only possible to understand and control glass corrosion through closely coupled theory, simulation, and experimentation. Improved understanding of the composition/structure effects on these processes would allow for rational design of glass waste forms with predictable long-term performance. The research will be conducted in three projects as shown in Figure 1. The three glass projects are R*ate-Limiting Mechanism of Glass Corrosion*; *Composition and Environmental Effects on Glass Corrosion Rate*; and *Rational Glass Design*.

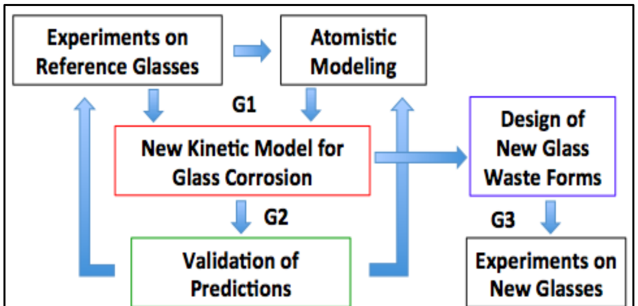

Fig. 1. Flow of glass projects.

Ceramics Projects

Not all of the DOE-EM wastes can be managed by bulk waste processing technology, as highly volatile components e.g., ^{129}I and $^{135}CsCl$ cannot be effectively incorporated into a borosilicate glass waste form. Single phase crystalline ceramics or multiphase assemblages have been investigated as alternative waste forms to borosilicate glass for high level waste (HLW), excess plutonium from dismantled nuclear weapons, and minor actinides separated during fuel reprocessing. The ceramics team targets fundamental understanding of radionuclide incorporation, confinement and transport behavior in bulk crystalline ceramics and across solid-solid and solid-liquid interfaces that can be closely linked with the ceramic waste form degradation and stability under near field conditions. The approach taken in this research is summarized in Figure 2. The two ceramics projects are: *Integrated Computation and Experimental Approach in Designing Waste Forms* and *Tailoring Performance and Degradation Mechanisms of Crystalline Waste Forms*.

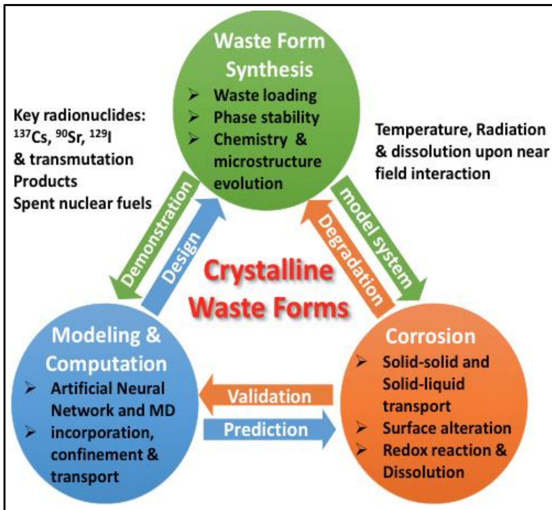

Fig. 2. Integrated approach for waste form design, evaluation and mechanistic understanding of crystalline ceramics

Metals Projects

Corrosion resistant alloys (CRAs) are used as materials of construction for canisters containing nuclear waste and have been proposed as waste forms for certain HLWs (e.g., pyrochemical metal wastes and isolated ^{99}Tc). CRAs are Fe- or Ni-based alloys that achieve their superior corrosion properties through the development of a thin protective surface oxide film, called a passive film. Unfortunately, CRAs are susceptible to rapid attack in the form of localized corrosion such as pitting, crevice corrosion, and stress corrosion cracking under conditions where the passive film breaks down locally. Improved CRAs could alter the nature and performance of any storage or disposal facility. The metals projects will study CRAs and use Integrated Computational Materials Engineering (ICME) to develop new and improved CRAs. This has never before been attempted. The two Metals projects are *Tailored Alloying in Corrosion Resistant Alloys (CRAs) and Development of New CRAs* and *Atmospheric Pitting and Cracking of Stainless Steels*.

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